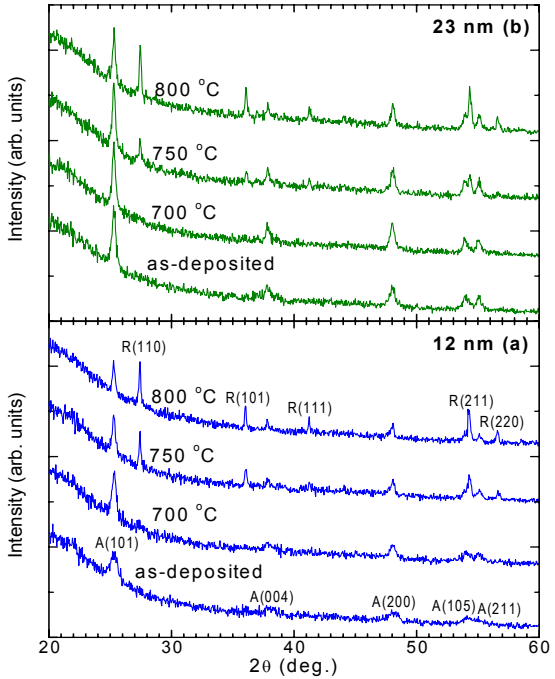
Observation of the Size Effect on Phase Transformation of TiO_2 Nanoparticles

- In order to design and control TiO_2 phase types and concentrations for more efficient photocatalysis. The phase transformation of TiO_2 nanoparticles with different sizes (12 nm, 17 nm, and 23 nm) was studied using XRD and TEM.
- The XRD results and the calculated activation energies are used to show the size dependence of phase transformation.



X-ray Diffraction Study of TiO_2 Phase Transformation

- XRD patterns from as-deposited samples and samples annealed at 700, 750, and 800 °C.
- The phase compositions were calculated based on formula

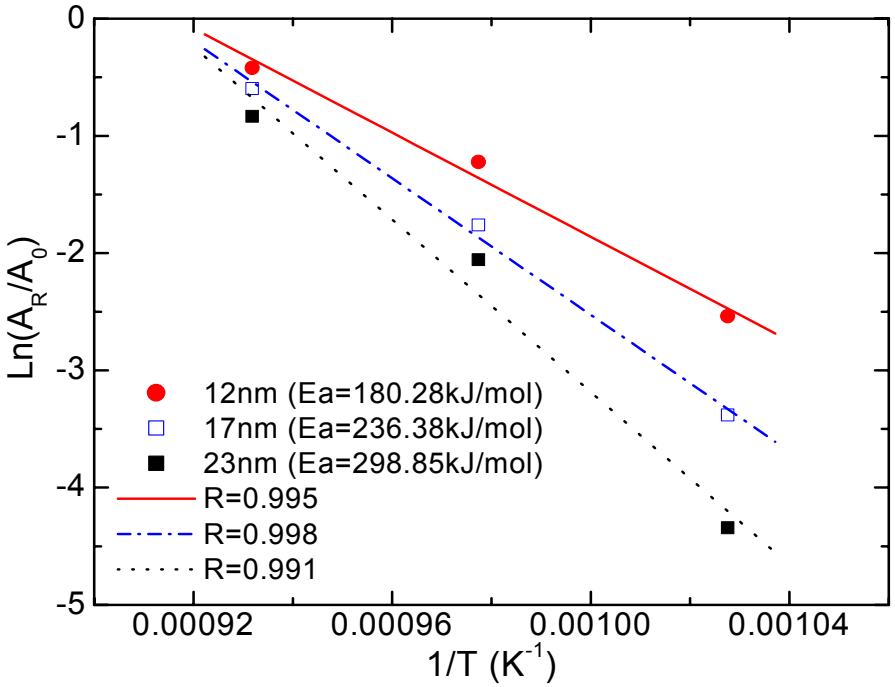
$$W_R = \frac{A_R}{A_0} = \frac{A_R}{0.884 A_A + A_R}$$

- Particle sizes were calculated.

(*)*A. A. Gribb and J. F. Banfield, Am. Mineral. 82, 717 (1997).*

Samples	$A_{R(110)}/(A_{R(110)}+0.884A_{A(101)})$ (±0.03)			
	As-deposited	700°C	750°C	800°C
12 nm	0	0.079	0.295	0.658
17 nm	0	0.034	0.172	0.551
23 nm	0	0.013	0.128	0.435

- Rutile and anatase relative phase concentrations calculated from XRD as functions of size and temperature.



Activation Energy Calculation

- $A_R=A_0Exp(-E_a/KT)$, $A_0=0.884A_A+A_R$
  E_a is anatase to rutile transformation activation energy.
- The activation energy decreases with the particle size and 12-nm sample has the lowest activation energy of 180.28 kJ/mol.

(*) *H. Zhang and J. F. Banfield, Am. Mineral.* ***84****, 528 (1999).*